Approximation of Bayesian Inverse Problems for PDEs

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Abstract

Inverse problems are often ill-posed, with solutions that depend sensitively on data. In any numerical approach to the solution of such problems, regularization of some form is needed to counteract the resulting instability. This paper is based on an approach to regularization, employing a Bayesian formulation of the problem, which leads to a notion of well-posedness for inverse problems, at the level of probability measures.

The stability which results from this well-posedness may be used as the basis for quantifying the approximation, in finite dimensional spaces, of inverse problems for functions. This paper contains a theory which utilizes the stability to estimate the distance between the true and approximate posterior distributions, in the Hellinger metric, in terms of error estimates for approximation of the underlying forward problem. This is potentially useful as it allows for the transfer of estimates from the numerical analysis of forward problems into estimates for the solution of the related inverse problem. In particular controlling differences in the Hellinger metric leads to control on the differences between expected values of polynomially bounded functions and operators, including the mean and covariance operator.

The ideas are illustrated with the classical inverse problem for the heat equation, and then applied to some more complicated non-Gaussian inverse problems arising in data assimilation, involving determination of the initial condition for the Stokes or Navier-Stokes equation from Lagrangian and Eulerian observations respectively.

1 Introduction

In applications it is frequently of interest to solve *inverse problems* [15, 26]: to find u, an input to a mathematical model, given y an observation of (some components of, or functions of) the solution of the model. We have an equation of the form

$$y = \mathcal{G}(u) \tag{1.1}$$

to solve for $u \in X$, given $y \in Y$, where X, Y are Banach spaces. We refer to evaluating $\mathcal{G}$ as solving the *forward problem*[1]. We refer to y as *data* or *observations*. It is typical of inverse problems that they are *ill-posed*: there may be no solution, or the solution may not be unique and may depend sensitively on y. For this reason some form of regularization is often employed [7] to stabilize computational approximations.

We adopt a Bayesian approach to regularization [2] which leads to the notion of finding a *probability measure* μ on X, containing information about the relative probability of different states u, given the data y. Adopting this approach is natural in situations where an analysis of the source of data reveals that the observations y are subject to noise. A more appropriate model equation is then often of the form

$$y = \mathcal{G}(u) + \eta \tag{1.2}$$

where η is a mean-zero random variable, whose statistical properties we might know, or make a reasonable mathematical model for, but whose actual value is unknown to us; we refer to η as the *observational noise*. We assume that it is possible to describe our prior knowledge about u, before acquiring data, in terms of a *prior probability measure* μ_0. It is then possible to use Bayes' formula to calculate the *posterior probability measure* μ for u given y.

In the infinite dimensional setting the most natural version of Bayes theorem is a statement that the posterior measure is absolutely continuous with respect to the prior [25] and that the Radon-Nikodym derivative (density) between them is determined by the data likelihood. This gives rise to the formula

$$\frac{d\mu}{d\mu_0}(u) = \frac{1}{Z(y)} \exp(-\Phi(u; y)) \tag{1.3}$$

where the *normalization constant* $Z(y)$ is chosen so that μ is a probability measure:

$$Z(y) = \int_X \exp(-\Phi(u; y)) d\mu_0(u). \tag{1.4}$$

[1] In the applications in this paper $\mathcal{G}$ is found from composition of the forward model with some form of observation operator, such as pointwise evaluation at a finite set of points. The resulting observation operator is often denoted with the letter $\mathcal{H}$ in the atmospheric sciences community [12]; because we need $\mathcal{H}$ for Hilbert space later on, we use the symbol $\mathcal{G}$.

In the case where y is finite dimensional and η has Lebesegue density ρ this is simply

$$\frac{d\mu}{d\mu_0}(u) \propto \rho(y - \mathcal{G}(u)). \tag{1.5}$$

More generally Φ is determined by the distribution of y given u. We call $\Phi(u; y)$ the *potential*, and sometimes, for brevity, refer to evaluation of $\Phi(u; y)$ for a particular $u \in X$, as *solving the forward problem* as it is defined through $\mathcal{G}(\cdot)$. Note that the solution to the inverse problem is a probability measure μ which is defined through a combination of solution of the forward problem $\mathcal{G}$, the data y and a prior probability measure μ_0.

In general it is hard to obtain information from a formula such as (1.3) for a probability measure. One useful approach to extracting information is to use *sampling*: generate a set of points $\{u^{(k)}\}_{k=1}^K$ distributed (perhaps only approximately) according to μ. In this context it is noteworthy that the integral $Z(y)$ appearing in formula (1.3) is not needed to enable implementation of MCMC methods to sample from the desired measure. These methods incur an error which is well understood and which decays as $\sqrt{K}$ [17]. However for inverse problems on function space there is a second source of error, arising from the need to approximate the inverse problem in a finite dimensional subspace of dimension N. The purpose of this paper is to quantify such approximation errors. The *key idea* is that we transfer approximation properties of the forward problem Φ into approximation properties of the inverse problem defined by (1.3).

Since the solution to the Bayesian inverse problem is a probability measure we will need to use metrics on probability measures to quantify the effect of approximation. We will employ the Hellinger metric d_{Hell} from Definition A.2 because this leads directly to bounds on the approximation error incurred when calculating the expectation of functions. This property is summarized in Lemma A.3. Combining these ideas we will find that finite dimensional approximation leads to an error in the calculation of expectation of functions which tends to zero as $\psi(N)$ tends to infinity, for some function $\psi(N)$ *determined by approximation of the forward problem.*

In section 2 we provide the general approximation theory, for measures μ given by (1.3), upon which the remainder of the paper builds. Section 3 employs this approximation theory to study the classical inverse problem of determining the initial condition for the heat equation from observation of the solution at a positive time. In section 4 we study the inverse problem of determining the initial condition for the Stokes equation, given a finite set of observations of Lagrangian trajectories defined through the time-dependent velocity field solving the Stokes equation; this section also includes numerical results showing the convergence of the posterior distribution under refinement of the finite dimensional approximation, as predicted by the theory. Section 5 is devoted to the related inverse

problem of determining the initial condition for the Navier-Stokes equation, given direct observation of the time-dependent velocity field at a finite set of points at positive times.

A classical approach to the regularization of inverse problems is through the least squares approach and Tikhonov regularization [7, 26]; a good overview of this approach, in the context of data assimilation problems in fluid mechanics such as those studied in sections 4 and 5, is [19] and the connection between the least squares and Bayesian approaches for applications in fluid mechanics is overviewed in [1]. The Bayesian formulation to inverse problems in general is overviewed in the text [14]. Note, however, that the methodology employed there is typically one in which the problem is first discretized, and then ideas from Bayesian statistics are applied to the resulting finite dimensional problem. The approach taken in this paper is to first formulate the Bayesian inverse problem *on function space* and then study approximation. As in many areas of applied mathematics – for example, optimal control – formulation of the problem in function space, followed by discretization will lead to better algorithms and better understanding. This approach is laid out conceptually in [26] for inverse problems, but the underlying mathematics is not developed, except for some particular linear and Gaussian problems. Indeed, for linear problems, the Bayesian approach on function space may be found in an early paper of Franklin [8], including study of the heat equation, the subject of section 3. More recently there has been some work on finite dimensional linear inverse problems, using the Bayesian approach to regularization, and considering infinite dimensional limits [10, 18] and in the limit of disappearing observational noise [11]. A general approach to the formulation, and well-posedness, of inverse problems, adopting a Bayesian approach on function space, is undertaken in [5]; furthermore applications to problems in fluid mechanics are given in that paper and we will build on this material in sections 4 and 5.

2 General Framework

In this section we establish three useful results which concern the effect of approximation on the posterior probability measure μ given by (1.3). These three results are Theorem 2.4, Corollary 2.5 and Theorem 2.6. The key point to notice about these results is that they simply require the proof of various bounds and approximation properties *for the forward problem*, and yet they yield approximation results concerning the Bayesian inverse problem. The connection to probability comes only through the choice of the space X, in which the bounds and approximation properties must be proved, which must have full measure under the prior μ_0.

The probability measure of interest (1.3) is defined through a density with respect to a prior reference measure μ_0 which, by shift of origin, we take to have mean zero. Furthermore, we assume that this reference measure is Gaussian with covariance operator $\mathcal{C}$. We write $\mu_0 = \mathcal{N}(0, \mathcal{C})$. In fact we only use the Fernique Theorem A.4 for μ_0 and the results may be trivially extended to all measures which satisfy the conclusion of this theorem. The Fernique Theorem holds for all Gaussian measures on a separable Banach space [3], and also for other measures with tails which decay at least as fast as a Gaussian.

It is demonstrated in [25] that in many applications, including those considered here, the potential $\Phi(\cdot; y)$ satisfies certain natural bounds on a Banach space $\Big(X, \|\cdot\|_X\Big)$, contained in the original Hilbert space on which μ_0 is defined, and of full measure under μ_0 so that $\mu_0(X) = 1$. Such bounds are summarized in the following assumptions. We assume that the data y lies in a Banach space $\Big(Y, \|\cdot\|_Y\Big)$. The key point about the form of Assumption 2.1(i) is that it allows use of the Fernique Theorem to control integrals against μ. The assumption (ii) may be used to obtain lower bounds on the normalization constant $Z(y)$.

Assumption 2.1 *For some Banach space X with $\mu_0(X) = 1$, the function $\Phi : X \times Y \to \mathbb{R}$ satisfies the following:*

i) for every $\varepsilon > 0$ and $r > 0$ there is $M = M(\varepsilon, r) \in \mathbb{R}$ such that, for all $u \in X$ and $y \in Y$ with $\|y\|_Y < r$,

$$\Phi(u; y) \geqslant M - \varepsilon \|u\|_X^2;$$

ii) for every $r > 0$ there is a $L = L(r) > 0$ such that, for all $u \in X$ and $y \in Y$ with $\max\{\|u\|_X, \|y\|_Y\} < r$,

$$\Phi(u; y) \leqslant L(r).$$

For Bayesian inverse problems in which a finite number of observations are made and the observation error η is mean zero Gaussian, the potential Φ has the form

$$\Phi(u; y) = \frac{1}{2}|y - \mathcal{G}(u)|_\Gamma^2 \tag{2.1}$$

where $y \in \mathbb{R}^m$ is the data, $\mathcal{G} : X \to \mathbb{R}^m$ is the forward model and $|\cdot|_\Gamma$ is a covariance weighted norm on $\mathbb{R}^m$ given by $|\cdot|_\Gamma = |\Gamma^{-\frac{1}{2}} \cdot|$ and $|\cdot|$ denotes the standard Euclidean norm. In this case it is natural to express conditions on the measure μ in terms of $\mathcal{G}$.

Assumption 2.2 *For some Banach space* X *with* $\mu_0(X) = 1$, *the function* $\mathcal{G} : X \to \mathbb{R}^m$ *satisfies the following: for every* $\varepsilon > 0$ *there is* $M = M(\varepsilon) \in \mathbb{R}$ *such that, for all* $u \in X$,

$$|\mathcal{G}(u)|_\Gamma \leqslant \exp(\varepsilon \|u\|_X^2 + M).$$

Lemma 2.3 *Assume that* $\Phi : X \times \mathbb{R}^m \to \mathbb{R}$ *is given by* (2.1) *and let* $\mathcal{G}$ *satisfy Assumptions 2.2. Assume also that* μ_0 *is a Gaussian measure satisfying* $\mu_0(X) = 1$. *Then* Φ *satisfies Assumptions 2.1.*

Proof. Assumption 2.1(i) is automatic since Φ is positive; assumption (ii) follows from the bound

$$\Phi(u; y) \leqslant |y|_\Gamma^2 + |\mathcal{G}(u)|_\Gamma^2$$

and use of the exponential bound on $\mathcal{G}$. □

Since the dependence on y is not relevant we suppress it notationally and study measures μ given by

$$\frac{d\mu}{d\mu_0}(u) = \frac{1}{Z} \exp(-\Phi(u)) \tag{2.2}$$

where the normalization constant Z is given by

$$Z = \int_X \exp(-\Phi(u)) d\mu_0(u). \tag{2.3}$$

We approximate μ by approximating Φ over some $N-$dimensional subspace of X. In particular we define μ^N by

$$\frac{d\mu^N}{d\mu_0}(u) = \frac{1}{Z^N} \exp(-\Phi^N(u)) \tag{2.4}$$

where

$$Z^N = \int_X \exp(-\Phi^N(u)) d\mu_0(u). \tag{2.5}$$

The potential Φ^N should be viewed as resulting from an approximation to the solution of the forward problem. Our interest is in translating approximation results for Φ into approximation results for μ.

The following theorem proves such a result, bounding the Hellinger distance, and hence by (A.6) the total variation distance, between measures μ and μ^N, in terms of the error in approximating Φ. Again the particular exponential dependence of the error constant for the forward approximation is required so that we may use the Fernique Theorem to control certain expectations arising in the analysis.

Theorem 2.4 *Assume that Φ and Φ^N satisfy Assumptions 2.1(i),(ii) with constants uniform in N. Assume also that, for any $\varepsilon > 0$, there is $K = K(\varepsilon) > 0$ such that*

$$|\Phi(u) - \Phi^N(u)| \leqslant K \exp(\varepsilon \|u\|_X^2)\psi(N) \tag{2.6}$$

where $\psi(N) \to 0$ as $N \to \infty$. Then the measures μ and μ^N are close with respect to the Hellinger distance: there is a constant C, independent of N, and such that

$$d_{\text{Hell}}(\mu, \mu^N) \leqslant C\psi(N). \tag{2.7}$$

Consequently all moments of $\|u\|_X$ are $\mathcal{O}(\psi(N))$ close. In particular the mean and, in the case X is a Hilbert space, the covariance operator, are $\mathcal{O}(\psi(N))$ close.

Proof. Throughout the proof, all integrals are over X. The constant C may depend upon r and changes from occurrence to occurrence. Using Assumption 2.1(ii) gives

$$|Z| \geqslant \int_{\{\|u\|_X \leqslant r\}} \exp(-L(r)) d\mu_0(u) \geqslant \exp(-L(r))\mu_0\{\|u\|_X \leqslant r\}.$$

This lower bound is positive because μ_0 has full measure on X and is Gaussian so that all balls in X have positive probability. We have an analogous lower bound for $|Z^N|$.

From Assumptions 2.1(i) and (2.6), using the fact that μ_0 is a Gaussian probability measure so that the Fernique Theorem A.4 applies,

$$\begin{aligned} |Z - Z^N| &\leqslant \int K\psi(N) \exp(\varepsilon\|u\|_X^2 - M) \exp(\varepsilon\|u\|_X^2) d\mu_0(u) \\ &\leqslant C\psi(N). \end{aligned}$$

From the definition of Hellinger distance we have

$$\begin{aligned} 2d_{\text{Hell}}(\mu, \mu^N)^2 &= \int \Big(Z^{-\frac{1}{2}} \exp(-\frac{1}{2}\Phi(u)) - (Z^N)^{-\frac{1}{2}} \exp(-\frac{1}{2}\Phi^N(u)) \Big)^2 d\mu_0(u) \\ &\leqslant I_1 + I_2 \end{aligned}$$

where

$$\begin{aligned} I_1 &= \frac{2}{Z} \int \Big(\exp(-\frac{1}{2}\Phi(u)) - \exp(-\frac{1}{2}\Phi^N(u)) \Big)^2 d\mu_0(u), \\ I_2 &= 2|Z^{-\frac{1}{2}} - (Z^N)^{-\frac{1}{2}}|^2 \int \exp(-\Phi^N(u)) d\mu_0(u). \end{aligned}$$

Now, again using Assumptions 2.1(i) and equation (2.6), together with the Fernique Theorem A.4,

$$\frac{Z}{2}I_1 \leqslant \int \frac{1}{4}K^2\psi(N)^2 \exp(3\varepsilon\|u\|_X^2 - M)d\mu_0(u)$$
$$\leqslant C\psi(N)^2.$$

Note that the bounds on Z, Z^N from below are independent of N. Furthermore,

$$\int \exp(-\Phi^N(u))d\mu_0(u) \leqslant \int \exp(\varepsilon\|u\|_X^2 - M)d\mu_0(u)$$

with bound independent of N, by the Fernique Theorem A.4. Thus

$$I_2 \leqslant C(Z^{-3} \vee (Z^N)^{-3})|Z - Z^N|^2$$
$$\leqslant C\psi(N)^2.$$

Combining gives the desired continuity result in the Hellinger metric.

Finally all moments of u in X are finite under the Gaussian measure μ_0 by the Fernique Theorem A.4. It follows that all moments are finite under μ and μ^N because, for $f : X \to Z$ polynomially bounded,

$$\mathbb{E}^\mu\|f\| \leqslant (\mathbb{E}^{\mu_0}\|f\|^2)^{\frac{1}{2}}(\mathbb{E}^{\mu_0}\exp(-2\Phi(u;y)))^{\frac{1}{2}}$$

and the first term on the right hand side is finite since all moments are finite under μ_0, whilst the second term may be seen to be finite by use of Assumption 2.1(i) and the Fernique Theorem A.4. □

For Bayesian inverse problems with finite data the potential Φ has the form given in (2.1) where $y \in \mathbb{R}^m$ is the data, $\mathcal{G} : X \to \mathbb{R}^m$ is the forward model and $|\cdot|_\Gamma$ is a covariance weighted norm on $\mathbb{R}^m$. In this context the following corollary is useful.

Corollary 2.5 *Assume that Φ is given by* (2.1) *and that $\mathcal{G}$ is approximated by a function $\mathcal{G}^N$ with the property that, for any $\varepsilon > 0$, there is $K' = K'(\varepsilon) > 0$ such that*

$$|\mathcal{G}(u) - \mathcal{G}^N(u)| \leqslant K' \exp(\varepsilon\|u\|_X^2)\psi(N) \tag{2.8}$$

where $\psi(N) \to 0$ as $N \to \infty$. If $\mathcal{G}$ and $\mathcal{G}^N$ satisfy Assumptions 2.2 uniformly in N then Φ and $\Phi^N := \frac{1}{2}|y - \mathcal{G}^N(u)|_\Gamma^2$ satisfy the conditions necessary for application of Theorem 2.4 and all the conclusions of that theorem apply.

Proof. That (i), (ii) of Assumptions 2.1 hold follows as in the proof of Lemma 2.3. Also (2.6) holds since (for some $K(\cdot)$ defined in the course of the following chain of inequalities)

$$\begin{aligned}|\Phi(u)-\Phi^N(u)| &\leqslant \frac{1}{2}|2y-\mathcal{G}(u)-\mathcal{G}^N(u)|_\Gamma|\mathcal{G}(u)-\mathcal{G}^N(u)|_\Gamma\\ &\leqslant \Big(|y|+\exp(\varepsilon\|u\|_X^2+M)\Big)\times K'(\varepsilon)\exp(\varepsilon\|u\|_X^2)\psi(N)\\ &\leqslant K(2\varepsilon)\exp(2\varepsilon\|u\|_X^2)\psi(N)\end{aligned}$$

as required. □

A notable fact concerning Theorem 2.4 is that the rate of convergence attained in the solution of the forward problem, encapsulated in approximation of the function Φ by Φ^N, is transferred into the rate of convergence of the related inverse problem for measure μ given by (2.2) and its approximation by μ^N. Key to achieving this transfer of rates of convergence is the dependence of the constant in the forward error bound (2.6) on u. In particular it is necessary that this constant is integrable by use of the Fernique Theorem A.4. In some applications it is not possible to obtain such dependence. Then convergence results can sometimes still be obtained, but at weaker rates. We now describe a theory for this situation.

Theorem 2.6 *Assume that Φ and Φ^N satisfy Assumptions 2.1(i),(ii) with constants uniform in N. Assume also that, for any $R>0$ there is $K=K(R)>0$ such that, for all u with $\|u\|_X\leqslant R$,*

$$|\Phi(u)-\Phi^N(u)|\leqslant K\psi(N) \tag{2.9}$$

where $\psi(N)\to 0$ as $N\to\infty$. Then the measures μ and μ^N are close with respect to the Hellinger distance:

$$d_{\text{Hell}}(\mu,\mu^N)\to 0 \tag{2.10}$$

as $N\to\infty$. Consequently all moments of $\|u\|_X$ under μ^N converge to corresponding moments under μ as $N\to\infty$. In particular the mean and, in the case X is a Hilbert space, the covariance operator, converge.

Proof. Throughout the proof, all integrals are over X unless specified otherwise. The constant C changes from occurrence to occurrence. The normalization constants Z and Z^N satisfy lower bounds which are identical to that proved for Z in the course of establishing Theorem 2.4.

From Assumptions 2.1(i) and (2.9),

$$\begin{aligned}
|Z - Z^N| &\leqslant \int_X |\exp(-\Phi(u)) - \exp(-\Phi^N(u))| d\mu_0 \\
&\leqslant \int_{\{\|u\|_X \leqslant R\}} \exp(\varepsilon \|u\|_X^2 - M) |\Phi(u) - \Phi^N(u)| d\mu_0(u) \\
&\quad + \int_{\{\|u\|_X > R\}} 2 \exp(\varepsilon \|u\|_X^2 - M) d\mu_0(u) \\
&\leqslant \exp(\varepsilon R^2 - M) K(R) \psi(N) + J_R \\
&:= K_1(R) \psi(N) + J_R.
\end{aligned}$$

Here

$$J_R = \int_{\{\|u\|_X > R\}} 2 \exp(\varepsilon \|u\|_X^2 - M) d\mu_0(u).$$

Now, again by the Fernique Theorem A.4, $J_R \to 0$ as $R \to \infty$ so, for any $\delta > 0$, we may choose $R > 0$ such that $J_R < \delta$. Now choose $N > 0$ so that $K_1(R)\psi(N) < \delta$ to deduce that $|Z - Z^N| < 2\delta$. Since $\delta > 0$ is arbitrary this proves that $Z^N \to Z$ as $N \to \infty$.

From the definition of Hellinger distance we have

$$\begin{aligned}
2 d_{\text{Hell}}(\mu, \mu^N)^2 &= \int \Big(Z^{-\frac{1}{2}} \exp(-\frac{1}{2}\Phi(u)) - (Z^N)^{-\frac{1}{2}} \exp(-\frac{1}{2}\Phi^N(u)) \Big)^2 d\mu_0(u) \\
&\leqslant I_1 + I_2
\end{aligned}$$

where

$$\begin{aligned}
I_1 &= \frac{2}{Z} \int \Big(\exp(-\frac{1}{2}\Phi(u)) - \exp(-\frac{1}{2}\Phi^N(u)) \Big)^2 d\mu_0(u), \\
I_2 &= 2 |Z^{-\frac{1}{2}} - (Z^N)^{-\frac{1}{2}}|^2 \int \exp(-\Phi^N(u)) d\mu_0(u).
\end{aligned}$$

Now, again using Assumptions 2.1(i) and equation (2.9),

$$\begin{aligned}
I_1 &\leqslant \frac{1}{2Z} \int_{\{\|u\|_X \leqslant R\}} K(R)^2 \psi(N)^2 \exp(\varepsilon \|u\|_X^2 - M) d\mu_0(u) \\
&\quad + \frac{4}{Z} \int_{\{\|u\|_X > R\}} 2 \exp(\varepsilon \|u\|_X^2 - M) d\mu_0(u) \\
&\leqslant \frac{1}{2Z} K_2(R) \psi(N)^2 + \frac{4}{Z} J_R,
\end{aligned}$$

for suitably chosen $K_2 = K_2(R)$. An argument similar to the one above for $|Z - Z^N|$ shows that $I_1 \to 0$ as $N \to \infty$.

Note that the bounds on Z, Z^N from below are independent of N. Furthermore,

$$\int \exp(-\Phi^N(u))d\mu_0(u) \leqslant \int \exp(\varepsilon\|u\|_X^2 - M)d\mu_0(u)$$

with bound independent of N, by the Fernique Theorem A.4. Thus

$$|Z^{-\frac{1}{2}} - (Z^N)^{-\frac{1}{2}}|^2 \leqslant C(Z^{-3} \vee (Z^N)^{-3})|Z - Z^N|^2$$

and so $I_2 \to 0$ as $N \to \infty$. Combining gives the desired continuity result in the Hellinger metric.

The proof may be completed by the same arguments used in Theorem 2.4.

□

3 The Heat Equation

Here we consider a problem where the solution of the heat equation is noisily observed at some fixed positive time $T > 0$. To be concrete we consider the heat equation on a bounded open set $D \subset \mathbb{R}^d$, with Dirichlet boundary conditions, and written as an ODE in Hilbert space $\mathcal{H} = L^2(D)$:

$$\frac{dv}{dt} + Av = 0, \quad v(0) = u. \tag{3.1}$$

Here $A = -\triangle$ with $D(A) = H_0^1(D) \bigcap H^2(D)$. We define the Sobolev spaces $\mathcal{H}^s$ as in (A.2) with $\mathcal{H} = \mathcal{H}^0 = L^2(D)$. We assume sufficient regularity conditions on D and its boundary ∂D to ensure that the operator A is the generator of an analytic semigroup and we use (A.4) without comment in what follows.

Assume that we observe the solution v at time T, subject to error in the form of a Gaussian random field, and that we wish to recover the initial condition u. This problem is classically ill-posed, because the heat equation is smoothing, and inversion of this operator is not continuous on any Sobolev space $\mathcal{H}^s$. Nonetheless, we will construct a well-defined Bayesian inverse problem. We state a theorem showing that the posterior measure is equivalent (in the sense of measures) to the prior measure and then study the effect of approximation via a spectral method in Theorem 3.3, showing that the approximation error in the inverse problem is exponentially small.

We place a prior measure on u which is a Gaussian measure $\mu_0 \sim \mathcal{N}(m_0, \mathcal{C}_0)$ with $\mathcal{C}_0 = \beta A^{-\alpha}$, for some $\beta > 0, \alpha > \frac{d}{2}$. The lower bound on α ensures that samples from the prior are continuous functions (Lemma A.5).

We assume that the observation is a function $y \in \mathcal{H}$ and we model it as

$$y = e^{-AT}u + \eta \tag{3.2}$$

where $\eta \sim \mathcal{N}(0, \mathcal{C}_1)$ and $\mathcal{C}_1 = \delta A^{-\gamma}$ for some $\delta > 0$ and $\gamma > d/2$ so that η is almost surely continuous, by Lemma A.5. The forward model $\mathcal{G} : \mathcal{H} \to \mathcal{H}$ is given by $\mathcal{G}(u) = e^{-AT}u$.

By conditioning the Gaussian random variable $(u, y) \in \mathcal{H} \times \mathcal{H}$ we find that the posterior measure for $u|y$ is also Gaussian $\mathcal{N}(m, \mathcal{C})$ with mean

$$m = m_0 + \frac{\beta}{\delta} e^{-AT} A^{\gamma-\alpha} \Big(I + \frac{\beta}{\delta} e^{-2AT} A^{\gamma-\alpha} \Big)^{-1} (y - e^{-AT} m_0) \tag{3.3}$$

and covariance operator

$$\mathcal{C} = \beta A^{-\alpha} \Big(I + \frac{\beta}{\delta} e^{-2AT} A^{\gamma-\alpha} \Big)^{-1}. \tag{3.4}$$

We can also derive a formula for the Radon-Nikodym derivative between $\mu(du) = \mathbb{P}(du|y)$ and the prior $\mu_0(du)$. We define $\Phi : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ by

$$\Phi(u; y) = \frac{1}{2} \| \mathcal{C}_1^{-\frac{1}{2}} e^{-AT} u \|^2 - \langle \mathcal{C}_1^{-\frac{1}{2}} e^{-AT} u, \mathcal{C}_1^{-\frac{1}{2}} y \rangle. \tag{3.5}$$

It is a straightforward application of the theory of Gaussian measures [3, 21], using the continuity properties of Φ established below, to prove the following:

Theorem 3.1 *[25] Consider the inverse problem for the initial condition u in* (3.1)*, subject to observation in the form* (3.2) *with observational noise $\eta \sim \mathcal{N}(0, \delta A^{-\gamma})$, $\delta > 0$ and $\gamma > \frac{d}{2}$. Assume that the prior measure is a Gaussian $\mu_0 = \mathcal{N}(m_0, \beta A^{-\alpha})$ with $m_0 \in \mathcal{H}^\alpha, \beta > 0$ and $\alpha > \frac{d}{2}$. Then the posterior measure μ is Gaussian with mean and variance determined by* (3.3) *and* (3.4)*. Furthermore, μ and the prior measure μ_0 are equivalent Gaussian measures with Radon-Nikodym derivative* (1.3) *given by* (3.5)*.*

Now we study the properties of Φ. To this end it is helpful to define, for any $\theta > 0$, the compact operator $K_\theta : \mathcal{H} \to \mathcal{H}$ given by

$$K_\theta := \mathcal{C}_1^{-\frac{1}{2}} e^{-\theta AT}.$$

Note that, for any $0 < \theta_1 < \theta_2 < \infty$ there is $C > 0$ such that, for all $u \in \mathcal{H}$,

$$\|K_{\theta_2} u\| \leqslant C \|K_{\theta_1} u\|.$$

Lemma 3.2 *The function $\Phi : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ satisfies Assumptions 2.1 with $X = Y = \mathcal{H}$ and, furthermore, for any $\varepsilon \in (0,1)$, there is $C = C(\varepsilon)$ such that*

$$|\Phi(u; y) - \Phi(v; y)| \leqslant C \Big(\|K_1 u\| + \|K_1 v\| + \|K_\varepsilon y\| \Big) \|K_{1-\varepsilon} u - K_{1-\varepsilon} v\|.$$

In particular, $\Phi(\cdot; y) : \mathcal{H} \to \mathbb{R}$ is continuous.

Proof. We may write

$$\Phi(u;y) = \frac{1}{2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-AT}u\|^2 - \langle \mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}u, \mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}y\rangle.$$

By the Cauchy-Schwarz inequality we have, for any $\delta > 0$,

$$\Phi(u;y) \geqslant -\frac{\delta^2}{2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}u\|^2 - \frac{1}{2\delta^2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}y\|^2$$

so that, by the compactness of $K_{\frac{1}{2}}$, Assumption 2.1(i) holds. Assumption 2.1(ii) holds, by a similar Cauchy-Schwarz argument, with

$$\Phi(u;y) \leqslant \frac{1}{2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-AT}u\|^2 + \frac{1}{2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}y\|^2 + \frac{1}{2}\|\mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}u\|^2$$

so that, by the compactness of K_θ,

$$\Phi(u;y) \leqslant C\Big(1 + \|u\|^2\Big). \tag{3.6}$$

Note that

$$\langle \mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}u, \mathcal{C}_1^{-\frac{1}{2}}e^{-\frac{1}{2}AT}y\rangle = \langle \mathcal{C}_1^{-\frac{1}{2}}e^{-(1-\varepsilon)AT}u, \mathcal{C}_1^{-\frac{1}{2}}e^{-\varepsilon AT}y\rangle.$$

Since Φ is quadratic in u the desired Lipschitz property holds. $\square$

Now we consider approximation of the posterior measure μ given by (3.5). Specifically we define P^N to be orthogonal projection in $\mathcal{H}$ into the subspace $\{\phi_k\}_{|k|\leqslant N}$ (a subset of the eigenfunctions of A as defined just before (A.1)) and define the measure μ^N given by

$$\frac{d\mu^N}{d\mu_0}(u) \propto \exp\Big(-\Phi(P^N u;y)\Big). \tag{3.7}$$

The measure μ^N is identical to μ_0 on the orthogonal complement of $P^N\mathcal{H}$. We now use the theory from the preceding section to estimate the distance between μ and μ^N.

Theorem 3.3 *There are constants $c_1 > 0, c_2 > 0$, independent of N, such that $d_{\text{Hell}}(\mu, \mu^N) \leqslant c_1\exp(-c_2N^2)$. Consequently the mean and covariance operator of μ and μ^N are $\mathcal{O}(\exp(-c_2N^2))$ close in the $\mathcal{H}$ and $\mathcal{H}-$operator norms respectively.*

Proof. We apply Theorem 2.4 with $X = \mathcal{H}$. By Lemma 3.2, together with the fact that $\|P^N u\| \leqslant \|u\|$, we deduce that Assumptions 2.1 hold for Φ and Φ^N, with constants independent of N. Furthermore, from the Lipschitz bound in Lemma 3.2, we have

$$|\Phi(u;y) - \Phi^N(u;y)| \leqslant C\Big(\|u\| + \|y\|\Big)\|K_{\frac{1}{2}}(u - P^N u)\|.$$

But

$$\|K_{\frac{1}{2}}(u - P^N u)\|^2 = \frac{1}{\delta}\sum_{|k|>N} \lambda_k^\gamma \exp(-\lambda_k T)|u_k|^2.$$

Since the eigenvalues λ_k grow like $|k|^2$, and since $x^\gamma \exp(-xT)$ is monotonic decreasing for x sufficiently large, we deduce that

$$\|K_{\frac{1}{2}}(u - P^N u)\|^2 \leqslant c_1 \exp(-c_2 N^2) \sum_{|k|>N} |u_k|^2 \leqslant c_1 \exp(-c_2 N^2)\|u\|^2.$$

The result follows (possibly by redefinition of c_1, c_2). □

4 Lagrangian Data Assimilation

In this section we turn to a non-Gaussian nonlinear example where the full power of the abstract theory is required. In oceanography a commonly used method of gathering data about ocean currents, temperature, salinity and so forth is through the use of Lagrangian instruments: objects transported by the fluid velocity field, which transmit positional information using GPS. The inverse problem termed *Lagrangian data assimilation* is to determine the velocity field in the ocean from the Lagrangian data [13, 16].

In this section we study an idealized model which captures the essence of Lagrangian data assimilation as practised in oceanography. For the fluid flow model we use the *Stokes equations*, describing incompressible Newtonian fluids at moderate Reynolds number. The real equations of oceanography are, of course, far more complex, requiring evolution of coupled fields for velocity, temperature and salinity. However the dissipative and incompressible nature of the flow field for the Stokes equations captures the key mathematical properties of ocean flows, and hence provides a useful simplified model.

We consider the incompressible Stokes equations written in the form:

$$\frac{\partial v}{\partial t} = \nu \Delta v - \nabla p + f, \quad (x,t) \in D \times [0,\infty), \tag{4.1a}$$

$$\nabla \cdot v = 0, \quad (x,t) \in D \times [0,\infty), \tag{4.1b}$$

$$v = u, \quad (x,t) \in \overline{D} \times \{0\}. \tag{4.1c}$$

Here D is the unit square. We impose periodic boundary conditions on the velocity field v and the pressure p. We assume that f has zero average over D, noting that this implies the same for $v(x,t)$, provided that $u(x) = v(x,0)$ has zero initial average. See [27, 28] for definitions of the Leray projector $P : L^2_{per} \to \mathcal{H}$ and Stokes operator A. We employ the Hilbert spaces $\{\mathcal{H}^s, \|\cdot\|_s\}$ defined by (A.2) and note that $\mathcal{H}^s = D(A^{s/2})$ for any $s > 0$.

The PDE can be formulated as a linear dynamical system on the Hilbert space

$$\mathcal{H} = \Big\{ u \in L^2_{\text{per}}(D) \Big| \int_D u dx = 0,\ \nabla \cdot u = 0 \Big\}, \tag{4.2}$$

with the usual $L^2(D)$ norm and inner-product on this subspace of $L^2_{\text{per}}(D)$. If we let $\psi = Pf$ then we may write the equation (4.1) as an ODE in Hilbert space $\mathcal{H}$:

$$\frac{dv}{dt} + \nu A v = \psi, \quad v(0) = u. \tag{4.3}$$

We assume that we are given noisy observations of J Lagrangian tracers with positions z_j solving the integral equations

$$z_j(t) = z_{j,0} + \int_0^t v(z_j(s), s) ds. \tag{4.4}$$

For simplicity assume that we observe all the tracers z at the same set of positive times $\{t_k\}_{k=1}^K$ and that the initial particle tracer positions $z_{j,0}$ are known to us:

$$y_{j,k} = z_j(t_k) + \eta_{j,k}, \quad j = 1, \dots, \mathrm{J} \;\; k = 1, \dots, \mathrm{K}, \tag{4.5}$$

where the $\eta_{j,k}$'s are zero mean Gaussian random variables. Concatenating data we may write

$$y = \mathcal{G}(u) + \eta \tag{4.6}$$

with $y = (y_{1,1}, \dots, y_{\mathrm{J,K}})^*$ and $\eta \sim \mathcal{N}(0, \Gamma)$ for some covariance matrix Γ capturing the correlations present in the noise. Note that $\mathcal{G}$ is a complicated function of the initial condition for the Stokes equations, describing the mapping from this initial condition into the positions of Lagrangian trajectories at positive times. We will show that the function $\mathcal{G}$ maps of $\mathcal{H}$ into $\mathbb{R}^{2\mathrm{JK}}$, and is continuous on a dense subspace of $\mathcal{H}$.

The objective of the inverse problem is to find the initial velocity field u, given y. We adopt a Bayesian approach and identify $\mu(du) = \mathbb{P}(u|y)du.$ We now spend some time developing the Bayesian framework, culminating in Theorem 4.3 which shows that μ is well-defined. The reader interested purely in approximation of μ can skip straight to Theorem 4.4.

The following result shows that the tracer equations (4.4) have a solution, under mild regularity assumptions on the initial data. An analogous result is proved in [6] for the case where the velocity field is governed by the Navier-Stokes equation and the proof may be easily extended to the case of the Stokes equations.

Theorem 4.1 *Let $\psi \in L^2(0,T;\mathcal{H})$ and let $v \in C([0,T];\mathcal{H})$ denote the solution of* (4.3) *with initial data $u \in \mathcal{H}$. Then the integral equation* (4.4) *has a unique solution $z \in C([0,T],\mathbb{R}^2)$.*

We assume throughout that ψ is sufficiently regular that this theorem applies. To determine a formula for the probability of u given y, we apply the Bayesian approach described in [5] for the Navier-Stokes equations, and easily generalized to the Stokes equations. For the prior measure we take $\mu_0 = \mathcal{N}(0, \beta A^{-\alpha})$ for some $\beta > 0, \alpha > 1$, with the condition on α chosen to ensure that draws from the prior are in $\mathcal{H}$, by Lemma A.5. We condition the prior on the observations, to find the *posterior* measure on u. The likelihood of y given u is

$$\mathbb{P}\,(y \mid u) \propto \exp\Big(-\frac{1}{2}|y-\mathcal{G}(u)|_\Gamma^2\Big).$$

This suggests the formula

$$\frac{d\mu}{d\mu_0}(u) \propto \exp\Big(-\Phi(u;y)\Big) \tag{4.7}$$

where

$$\Phi(u;y) := \frac{1}{2}|y-\mathcal{G}(u)|_\Gamma^2 \tag{4.8}$$

and μ_0 is the prior Gaussian measure. We now make this assertion rigorous. The first step is to study the properties of the forward model $\mathcal{G}$. Proof of the following lemma is given after statement and proof of the main approximation result, Theorem 4.4.

Lemma 4.2 *Assume that $\psi \in C([0,T];\mathcal{H}^\gamma)$ for some $\gamma \geqslant 0$. Consider the forward model $\mathcal{G} : \mathcal{H} \to \mathbb{R}^{2JK}$ defined by* (4.5),(4.6).

- *If $\gamma \geqslant 0$ then, for any $\ell \geqslant 0$ there is $C > 0$ such that, for all $u \in \mathcal{H}^\ell$,*

$$|\mathcal{G}(u)| \leqslant C(1 + \|u\|_\ell).$$

- *If $\gamma > 0$ then, for any $\ell > 0$ and $R > 0$ and for all u_1, u_2 with $\|u_1\|_\ell \vee \|u_2\|_\ell < R$, there is $L = L(R) > 0$ such that*

$$|\mathcal{G}(u_1) - \mathcal{G}(u_2)| \leqslant L\|u_1 - u_2\|_\ell.$$

Furthermore, for any $\varepsilon > 0$, there is $M > 0$ such that $L(R) \leqslant M\exp(\varepsilon R^2)$.

Thus $\mathcal{G}$ satisfies Assumptions 2.2 with $X = \mathcal{H}^s$ and any $s \geqslant 0$.

Since $\mathcal{G}$ is continuous on $\mathcal{H}^\ell$ for $\ell > 0$ and since, by Lemma A.5, draws from μ_0 are almost surely in $\mathcal{H}^s$ for any $s < \alpha - 1$, use of the techniques in [5], employing the Stokes equation in place of the Navier-Stokes equation, shows the following:

Theorem 4.3 *Assume that $\psi \in C([0,T];\mathcal{H}^\gamma)$, for some $\gamma > 0$, and that the prior measure $\mu_0 = \mathcal{N}(0, \beta\mathcal{A}^{-\alpha})$ is chosen with $\beta > 0$ and $\alpha > 1$. Then the measure $\mu(du) = \mathbb{P}(du|y)$ is absolutely continuous with respect to the prior $\mu_0(du)$, with Radon-Nikodym derivative given by* (4.7).

In fact the theory in [5] may be used to show that the measure μ is Lipschitz in the data y, in the Hellinger metric. This well-posedness underlies the following study of the approximation of μ in a finite dimensional space. We define P^N to be orthogonal projection in $\mathcal{H}$ into the subspace $\{\phi_k\}_{|k| \leqslant N}$; recall that $k \in \mathbb{K} := \mathbb{Z}^2 \backslash \{0\}$. Since P^N is an orthogonal projection in any $\mathcal{H}^a$ we have $\|P^N u\|_X \leqslant \|u\|_X$. Define

$$\mathcal{G}^N(u) := \mathcal{G}(P^N u).$$

The approximate posterior measure μ^N is given by (4.7) with $\mathcal{G}$ replaced by $\mathcal{G}^N$. As in the last section it is identical to the prior on the orthogonal complement of $P^N\mathcal{H}$. On $P^N\mathcal{H}$ itself the measure is finite dimensional and amenable to sampling techniques as demonstrated in [4]. We now quantify the error arising from approximation of $\mathcal{G}$ in the finite dimensional subspace $P^N X$.

Theorem 4.4 *Let the assumptions of Theorem 4.3 hold. Then, for any $q < \alpha - 1$, there is a constant $c > 0$, independent of N, such that $d_{\text{Hell}}(\mu, \mu^N) \leqslant cN^{-q}$. Consequently the mean and covariance operator of μ and μ^N are $\mathcal{O}(N^{-q})$ close in the $\mathcal{H}$ and $\mathcal{H}-$operator norms respectively.*

Proof. We set $X = \mathcal{H}^s$ for any $s \in (0, \alpha - 1)$. We employ Corollary 2.5. Clearly, since $\mathcal{G}$ satisfies Assumptions 2.2 by Lemma 4.2, so too does $\mathcal{G}^N$, with constants uniform in N. It remains to establish (2.8). Write $u \in \mathcal{H}^s$ as

$$u = \sum_{k \in \mathbb{K}} u_k \phi_k$$

and note that

$$\sum_{k \in \mathbb{K}} |k|^{2s} |u_k|^2 < \infty.$$

We have, for any $\ell \in (0, s)$,

$$
\begin{aligned}
\|u - P^N u\|_\ell^2 &= \sum_{|k|>N} |k|^{2\ell} |u_k|^2 \\
&= \sum_{|k|>N} |k|^{2(\ell-s)} |k|^{2s} |u_k|^2 \\
&\leqslant N^{-2(s-\ell)} \sum_{|k|>N} |k|^{2s} |u_k|^2 \\
&\leqslant C\|u\|_s^2 N^{-2(s-\ell)}.
\end{aligned}
$$

By the Lipschitz properties of $\mathcal{G}$ from Lemma 4.2 we deduce that, for any $\ell \in (0, s)$,

$$
\begin{aligned}
|\mathcal{G}(u) - \mathcal{G}(P^N u)| &\leqslant M \exp(\varepsilon \|u\|_\ell^2) \|u - P^N u\|_\ell \\
&\leqslant C^{\frac{1}{2}} M \exp(\varepsilon \|u\|_s^2) \|u\|_s N^{-(s-\ell)}.
\end{aligned}
$$

This establishes the desired error bound (2.8). It follows from Corollary 2.5 that μ^N is $\mathcal{O}(N^{-(s-\ell)})$ close to μ in the Hellinger distance. Choosing s arbitrarily close to its upper bound, and ℓ arbitrarily close to zero, yields the optimal exponent q as appears in the theorem statement. $\square$

Proof. of Lemma 4.2 Throughout the proof, the constant C may change from instance to instance, but is always independent of the u_i. It suffices to consider a single observation so that $J = K = 1$. Let $z^{(i)}(t)$ solve

$$
z^{(i)}(t) = z_0^{(i)} + \int_0^t v^{(i)}(z^{(i)}(\tau), \tau) d\tau
$$

where $v^{(i)}(x, t)$ solves (4.1) with $u = u_i$.

Let $\ell \in [0, 2 + \gamma)$. Recall that, by (A.5),

$$
\|v^{(i)}(t)\|_s \leqslant C\Big(\frac{1}{t^{(s-\ell)/2}} \|u_i\|_\ell + \|\psi\|_{C([0,T];\mathcal{H}^\gamma)}\Big), \tag{4.9}
$$

for $s \in [\ell, 2 + \gamma)$. Also, by linearity and (A.4),

$$
\|v^{(1)}(t) - v^{(2)}(t)\|_s \leqslant \frac{C}{t^{(s-\ell)/2}} \|u_1 - u_2\|_\ell. \tag{4.10}
$$

To prove the first part of the lemma note that, by the Sobolev embedding The-

orem, for any $s > 1$,

$$\begin{aligned}
|z^{(i)}(t)| &\leqslant |z_0^{(i)}| + \int_0^t \|v^{(i)}(\cdot,\tau)\|_{L^\infty} d\tau \\
&\leqslant C\Big(1 + \int_0^t \|v^{(i)}(\cdot,\tau)\|_s d\tau\Big) \\
&\leqslant C\Big(1 + \int_0^t \frac{1}{\tau^{(s-\ell)/2}} \|u_i\|_\ell d\tau\Big).
\end{aligned}$$

For any $\gamma \geqslant 0$ and $\ell \in [0, 2+\gamma)$ we may choose s such that $s \in [\ell, 2+\gamma) \bigcap (1, \ell + 2)$. Thus the singularity is integrable and we have, for any $t \geqslant 0$,

$$|z^{(i)}(t)| \leqslant C(1 + \|u_i\|_\ell)$$

as required.

To prove the second part of the lemma choose $\ell \in (0, 2+\gamma)$ and then choose $s \in [\ell-1, 1+\gamma) \cap (1, \ell+1)$; this requires $\gamma > 0$ to ensure a nonempty intersection. Then

$$\|v^{(i)}(t)\|_{1+s} \leqslant C\Big(\frac{1}{t^{(1+s-\ell)/2}} \|u_i\|_\ell + \|\psi\|_{C([0,T];\mathcal{H}^\gamma)}\Big). \tag{4.11}$$

Now we have

$$\begin{aligned}
|z^{(1)}(t) - z^{(2)}(t)| &\leqslant |z^{(1)}(0) - z^{(2)}(0)| + \int_0^t |v^{(1)}(z^{(1)}(\tau),\tau) - v^{(2)}(z^{(2)}(\tau),\tau)| d\tau \\
&\leqslant \int_0^t \|Dv^{(1)}(\cdot,\tau)\|_{L^\infty} |z^{(1)}(\tau) - z^{(2)}(\tau)| d\tau \\
&\quad + \int_0^t \|v^{(1)}(\cdot,\tau) - v^{(2)}(\cdot,\tau)\|_{L^\infty} d\tau \\
&\leqslant \int_0^t \|v^{(1)}(\cdot,\tau)\|_{1+s} |z^{(1)}(\tau) - z^{(2)}(\tau)| d\tau \\
&\quad + \int_0^t \|v^{(1)}(\cdot,\tau) - v^{(2)}(\cdot,\tau)\|_s d\tau \\
&\leqslant \int_0^t C\Big(\frac{1}{\tau^{(1+s-\ell)/2}} \|u_1\|_\ell + \|\psi\|_{C([0,T];\mathcal{H}^\gamma)}\Big) |z^{(1)}(\tau) - z^{(2)}(\tau)| d\tau \\
&\quad + \int_0^t \frac{C}{\tau^{(s-\ell)/2}} \|u_1 - u_2\|_\ell d\tau.
\end{aligned}$$

Both time singularities are integrable and application of the Gronwall inequality from Lemma A.1 gives, for some C depending on $\|u_1\|_\ell$ and $\|\psi\|_{C([0,T];\mathcal{H}^\gamma)}$,

$$\|z^{(1)} - z^{(2)}\|_{L^\infty((0,T);\mathbb{R}^2)} \leqslant C\|u_1 - u_2\|_\ell.$$

The desired Lipschitz bound on $\mathcal{G}$ follows. In particular, the desired dependence of the Lipschitz constant follows from the fact that, for any $\varepsilon > 0$ there is $M > 0$ with the property that, for all $\theta \geqslant 0$,

$$1 + \theta \exp(\theta) \leqslant M \exp(\varepsilon\theta^2).$$

□

We conclude this section with the results of numerical experiments illustrating the theory. We compute the posterior distribution on the initial condition for Stokes equations from observation of J Lagrangian trajectories at one time $t = 0.1$. The prior measure is taken to be $\mathcal{N}(0, 400 \times A^{-2})$. The initial condition used to generate the data is found by making a single draw from the prior measure and the observational noise on the Lagrangian data is i.i.d $\mathcal{N}(0, \gamma^2)$ with $\gamma = 0.01$.

Note that, in the periodic geometry assumed here, the Stokes equations can be solved exactly by Fourier analysis [28]. Thus there are four sources of approximation when attempting to sample the posterior measure on u. These are

- (i) the effect of generating approximate samples from the posterior measure by use of MCMC methods;
- (ii) the effect of approximating u in a finite space found by orthogonal projection on the eigenbasis of the Stokes operator;
- (iii) the effect of interpolating a velocity field on a grid, found from use of the FFT, into values at the arbitrary locations of Lagrangian tracers;
- (iv) the effect of time-step in an Euler integration of the Lagrangian trajectory equations.

The MCMC method that we use is a generalization of the random walk Metropolis method and is detailed in [4]. The method is appropriate for sampling measures absolutely continuous with respect to a Gaussian in the situation where it is straightforward to sample directly from the Gaussian itself. We control the error (i) simply by running the MCMC method until time averages of various test statistics have converged; the reader interested in the effect of this Monte Carlo error should consult [4]. The error in (ii) is precisely the error which we quantify in Theorem 4.4; for the particular experiments used here we predict an error of order N^{-q} for any $q \in (0, 1)$. In this paper we have not analyzed the errors resulting from (iii) and (iv): these approximations are not included in the analysis leading to Theorem 4.4. However we anticipate that Theorem 2.4 or Theorem 2.6 could be used to study such approximations and the numerical evidence which follows below is consistent with this conjecture.

In the following three numerical experiments (each illustrated by a figure) we study the effect of one or more of the approximations (ii), (iii) and (iv) on the empirical distribution ('histogram') found from marginalizing data from the MCMC method onto the real part of the Fourier mode with wavevector $k = (0, 1)$. Similar results are found for other Fourier modes although it is important to note that at high values of $|k|$ the data is uninformative and the posterior is very close to the prior (see [4] for details). The first two figures use $J = 9$ Lagrangian trajectories, whilst the third uses $J = 400$. Figure 1 shows the effect of increasing the number of Fourier modes[2] used from 16, through 100 and 196, to a total of 400 modes and illustrates Theorem 4.4 in that convergence to a limit is observed as the number of Fourier modes increases. However this experiment is conducted by using

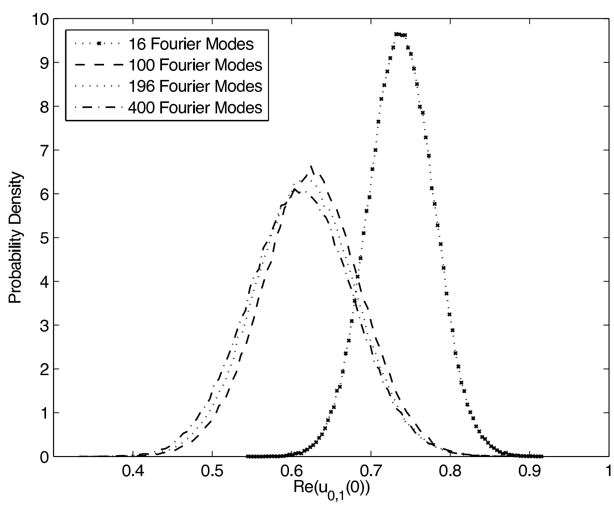

Figure 1: Marginal distributions on Re($u_{0,1}(0)$) with differing numbers of Fourier modes.

bilinear interpolation of the velocity field on the grid, in order to obtain off-grid velocities required for particle trajectories. At the cost of quadrupling the number of FFTs it is possible to implement bicubic interpolation [3]. Conducting the same refinement of the number of Fourier modes then yields Figure 2. Comparison of Figures 1 and 2 shows that the approximation (iii) by increased order of interpolation leads to improved approximation of the posterior distribution, and Figure 2

[2]Here by number of Fourier modes, we mean the dimension of the Fourier space approximation, ie then number of grid points

[3]Bicubic interpolation with no added FFTs is also possible by using finite difference methods to find the partial derivatives, but at a lower order of accuracy

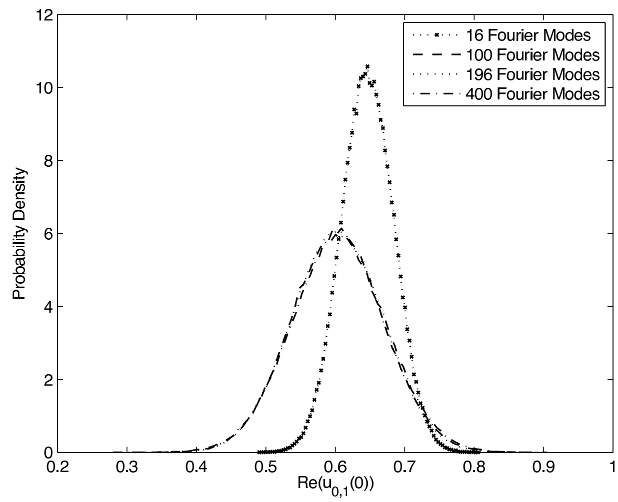

Figure 2: Marginal distributions on Re($u_{0,1}(0)$) with differing numbers of Fourier modes, bicubic interpolation used.

alone again illustrates Theorem 4.4. Figure 3 shows the effect (iv) of reducing the time-step used in the integration of the Lagrangian trajectories. Note that many more (400) particles were used to generate the observations leading to this figure than were used in the preceding two figures. This explains the quantitatively different posterior distribution; in particular the variance in the posterior distribution is considerably smaller. The result shows clearly that reducing the time-step leads to convergence in the posterior distribution.

5 Eulerian Data Assimilation

In this section we consider a data assimilation problem that is related to weather forecasting applications. In this problem, direct observations are made of the velocity field of an incompressible viscous flow at some fixed points in space-time, the mathematical model is the two-dimensional Navier-Stokes equations on a torus, and the objective is to obtain an estimate of the initial velocity field. The spaces $\mathcal{H}$ and $\mathcal{H}^s$ are as defined in Section 4, with $\|\cdot\|_s$ the norm in $\mathcal{H}^s$ and $\|\cdot\| = \|\cdot\|_0$. The definitions of A, the Stokes operator, and P, the Leray projector, are also as in the previous section [27, 28].

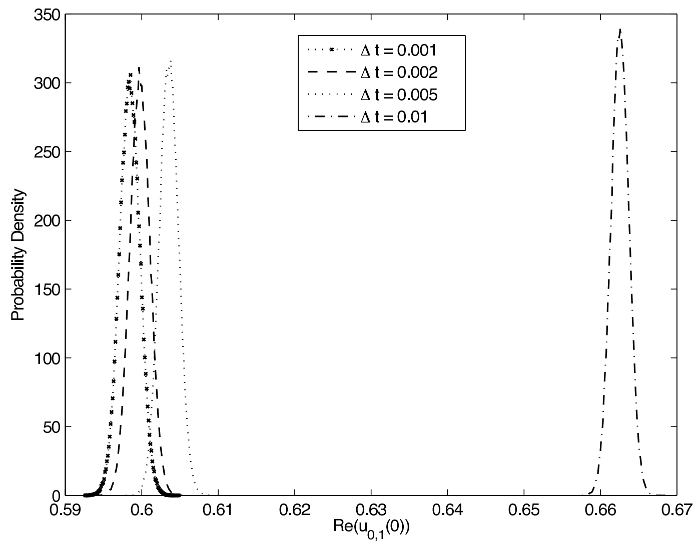

Figure 3: Marginal distributions on Re($u_{0,1}(0)$) with differing timestep, Lagrangian data

We consider the incompressible two-dimensional Navier-Stokes equations

$$\begin{aligned}\frac{\partial v}{\partial t} = \nu\Delta v - (v\cdot\nabla)v - \nabla p + f, &\quad (x,t)\in D\times[0,\infty),\\ \nabla\cdot v = 0, &\quad (x,t)\in D\times[0,\infty),\\ v = u, &\quad (x,t)\in \overline{D}\times\{0\},\end{aligned}$$

where D is a unit square as before and the boundary conditions are periodic. We apply the Leray Projector $P : L^2_{per}(D) \to \mathcal{H}$ and write the Navier-Stokes equations as an ordinary differential equation in $\mathcal{H}$

$$\frac{\mathrm{d}v}{\mathrm{d}t} + \nu A v + B(v,v) = \psi, \quad v(0) = u \tag{5.1}$$

with A the Stokes operator, $B(v,v) = P((v\cdot\nabla)v)$ and $\psi = Pf$.

For simplicity we assume that we make noisy observations of the velocity field v at time $t>0$ and at points $x_1,\dots,x_K \in D$:

$$y_k = v(x_k,t) + \eta_k, \quad k = 1,\dots,K.$$

We assume that the noise is Gaussian and the η_k form an i.i.d sequence with $\eta_1 \sim \mathcal{N}(0,\gamma^2)$. It is known (see Chapter 3 of [27], for example) that for $u \in \mathcal{H}$ and

$f \in L^2(0, T; \mathcal{H}^s)$ with $s > 0$ a unique solution to (5.1) exists which satisfies $u \in L^\infty(0, T; \mathcal{H}^{1+s}) \subset L^\infty(0, T; L^\infty(D))$. Therefore for such initial condition and forcing function the value of v at any $x \in D$ can be written as a function of u. Hence, we can write

$$y = \mathcal{G}(u) + \eta$$

where $y = (y_1, \cdots, y_{\mathrm{K}})^T \in \mathbb{R}^{\mathrm{K}}$ and $\eta = (\eta_1, \ldots, \eta_k)^T \in \mathbb{R}^{\mathrm{K}}$ is distributed as $\mathcal{N}(0, \gamma^2 I)$ and

$$\mathcal{G}(u) = (v(x_1, t), \cdots, v(x_{\mathrm{K}}, t))^T. \tag{5.2}$$

Now consider a Gaussian prior measure $\mu_0 \sim \mathcal{N}(u_b, \beta A^{-\alpha})$ with $\beta > 0$ and $\alpha > 1$; recall that the second condition ensures that functions drawn from the prior are in $\mathcal{H}$, by Lemma A.5. In Theorem 3.4 of [5] it is shown that with such prior measure, the posterior measure of the above inverse problem is well-defined:

Theorem 5.1 *Assume that $f \in L^2(0, T, \mathcal{H}^s)$ with $s > 0$. Consider the Eulerian data assimilation problem described above. Define a Gaussian measure μ_0 on $\mathcal{H}$, with mean u_b and covariance operator $\beta\, A^{-\alpha}$ for any $\beta > 0$ and $\alpha > 1$. If $u_b \in \mathcal{H}^\alpha$, then the probability measure $\mu(du) = \mathbb{P}(du|y)$ is absolutely continuous with respect to μ_0 with Radon-Nikodym derivative*

$$\frac{d\mu}{d\mu_0}(u) \propto \exp\left(-\frac{1}{2\gamma^2}|y - \mathcal{G}(u)|_\Sigma^2\right). \tag{5.3}$$

We now define an approximation μ^N to μ given by (5.3). The approximation is made by employing the Galerkin approximations of v to define an approximate $\mathcal{G}$. The Galerkin approximation of v, v^N, is the solution of

$$\frac{\mathrm{d}v^N}{\mathrm{d}t} + \nu A v^N + P^N B(v^N, v^N) = P^N \psi, \quad v^N(0) = P^N u, \tag{5.4}$$

with P^N as defined in the previous section. Let

$$\mathcal{G}^N(u) = (v^N(x_1, t), \ldots, v^N(x_K, t))^T$$

and then consider the approximate prior measure μ^N defined via its Radon-Nikodym derivative with respect to μ_0:

$$\frac{d\mu^N}{d\mu_0} \propto \exp\left(-\frac{1}{2\gamma^2}|y - \mathcal{G}^N(u)|_\Sigma^2\right). \tag{5.5}$$

Our aim is to show that μ^N converges to μ in the Hellinger metric. Unlike the examples in the previous two sections we are unable to obtain sufficient control

on the dependence of the error constant on u in the forward error bound to enable application of Theorem 2.4; hence we employ Theorem 2.6. In the following lemma we obtain a bound on $\|v(t)-v^N(t)\|_{L^\infty(D)}$ and therefore on $|\mathcal{G}(u)-\mathcal{G}^N(u)|$. Following the statement of the lemma, we state and prove the basic approximation theorem for this section. The proof of the lemma is given after the statement and proof of the approximation theorem for the posterior probability measure.

Lemma 5.2 *Let v^N be the solution of the Galerkin system (5.4). For any $t > t_0$*

$$\|v(t) - v^N(t)\|_{L^\infty(D)} \leqslant C(\|u\|, t_0)\, \psi(N),$$

where $\psi(N) \to 0$ as $N \to \infty$.

The above lemma leads us to the following convergence result for μ^N:

Theorem 5.3 *Let μ^N be defined according to (5.5) and let the assumptions of Theorem 5.1 hold. Then*

$$d_{\text{Hell}}(\mu, \mu^N) \to 0$$

as $N \to \infty$.

Proof. We apply Theorem 2.6 with $X = \mathcal{H}$. Assumption 2.2 (and hence Assumption 2.1) is established in Lemma 3.1 of [5]. By Lemma 5.2

$$|\mathcal{G}(u) - \mathcal{G}^N(u)| \leqslant K\psi(N)$$

with $K = K(\|u\|)$ and $\psi(N) \to 0$ as $N \to 0$. Therefore the result follows by Theorem 2.6. □

Proof of Lemma 5.2. Let $e_1 = v - P^N v$ and $e_2 = P^N v - v^N$. Applying P^N to (5.1) yields

$$\frac{\mathrm{d}P^N v}{\mathrm{d}t} + \nu A P^N v + P^N B(v, v) = P^N \psi.$$

Therefore $e_2 = P^N v - v^N$ satisfies

$$\frac{\mathrm{d}e_2}{\mathrm{d}t} + \nu A e_2 = P^N B(e_1 + e_2, v) + P^N B(v^N, e_1 + e_2), \quad e_2(0) = 0. \tag{5.6}$$

Since for any and for $m > l$

$$\|e_1\|_l^2 \leqslant \frac{1}{N^{2(m-l)}} \|v\|_m^2, \tag{5.7}$$

we will obtain an upper bound for $\|e_2\|_{1+l}$, $l > 0$, in terms of the Sobolev norms of e_1 and then use the embedding $\mathcal{H}^{1+l} \subset L^\infty$ to conclude the result of the lemma.

Taking the inner product of (5.6) with e_2, and noting that P^N is self-adjoint and $P^N e_2 = e_2$ and $(B(v,w),w) = 0$, we obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|e_2\|^2 + \nu\|De_2\|^2 &= (B(e_1+e_2,v),e_2) + (B(v^N,e_1),e_2)\\ &\leqslant c\|e_1\|^{1/2}\|e_1\|_1^{1/2}\|v\|_1\|e_2\|^{1/2}\|e_2\|_1^{1/2} + c\|e_2\|\,\|v\|_1\,\|e_2\|_1\\ &\quad + c\|v^N\|^{1/2}\|v^N\|_1^{1/2}\|e_1\|_1\|e_2\|^{1/2}\|e_2\|_1^{1/2}\\ &\leqslant c\|e_1\|^2\,\|e_1\|_1^2 + c\|v\|_1^2\,\|e_2\| + c\|e_2\|^2\,\|v\|_1^2\\ &\quad + c\|v^N\|\,\|v^N\|_1\,\|e_1\|_1 + c\|e_1\|_1\,\|e_2\| + \frac{\nu}{2}\|e_2\|_1^2\end{aligned}$$

Therefore

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}(1+\|e_2\|^2) + \nu\,\|De_2\|^2 \leqslant\\ &\qquad c\,(1+\|v\|_1^2)\,(1+\|e_2\|^2) + c(1+\|e_1\|^2)\,\|e_1\|_1^2 + c\,\|v^N\|\,\|v^N\|_1\,\|e_1\|_1\end{aligned}$$

which gives

$$\begin{aligned}\|e_2(t)\|^2 + \nu\int_0^t \|De_2\|^2 &\leqslant c\,\beta(t)\left(1+\int_0^t \|v^N\|^2\,\|v^N\|_1^2\,\mathrm{d}\tau\right)\int_0^t \|e_1\|_1^2\,\mathrm{d}\tau\\ &\quad + c\,\beta(t)\int_0^t (1+\|e_1\|^2)\,\|e_1\|_1^2\,\mathrm{d}\tau.\end{aligned}$$

with

$$\beta(t) = \exp\left(c\int_0^t 1+\|v\|_1^2\,\mathrm{d}\tau\right).$$

Hence

$$\|e_2(t)\|^2 + \nu\int_0^t \|De_2\|^2 \leqslant c(1+\|u\|^4)\,\mathrm{e}^{c+c\|u\|^2}\int_0^t (1+\|e_1\|^2)\,\|e_1\|_1^2\,\mathrm{d}\tau. \quad (5.8)$$

To estimate $\|e_2(t)\|_s$ for $s < 1$, we take the inner product of (5.6) with $A^s e_2$, $0 < s < 1$ and write

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|e_2\|_s^2 + \nu\|e_2\|_{1+s}^2 \leqslant |(((e_1+e_2)\cdot\nabla)v, A^s e_2)| + |((v^N\cdot\nabla)(e_1+e_2), A^s e_2)|.$$

Using

$$|((u\cdot\nabla)v, A^s w)| \leqslant c\|u\|_s\,\|v\|_1\,\|w\|_{1+s}$$

and Young's inequality we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\|e_2\|_s^2 + \nu\|e_2\|_{1+s}^2 \leqslant c\,(\|e_1\|_s^2 + \|e_2\|_s^2)\,\|v\|_1^2 + c\,\|v^N\|_s^2\,(\|e_1\|_1^2 + \|e_2\|_1^2).$$

Now integrating with respect to t over (t_0, t) with $0 < t_0 < t$ we can write

$$\|e_2(t)\|_s^2 + \nu \int_{t_0}^t \|e_2\|_{1+s}^2 \, \mathrm{d}\tau \leqslant \|e_2(t_0)\|_s^2 + c \sup_{\tau \geqslant t_0} \|v(\tau)\|_1^2 \int_0^t \|e_1\|_s^2 + \|e_2\|_s^2 \mathrm{d}\tau + c \sup_{\tau \geqslant t_0} \|v^N(\tau)\|_s^2 \int_0^t \|e_1\|_1^2 + \|e_2\|_1^2 \, \mathrm{d}\tau.$$

Therefore since for $s \leqslant 1$ and $t \geqslant t_0$

$$\|v(t)\|_s^2 \leqslant \frac{c(1 + \|u\|^2)}{t_0^s},$$

and noting that the same kind of decay bounds that hold for v can be shown similarly for v^N as well, we have

$$\|e_2(t)\|_s^2 + \nu \int_{t_0}^t \|e_2\|_{1+s}^2 \, \mathrm{d}\tau \leqslant \|e_2(t_0)\|_s^2 + \frac{c}{t_0}(1 + \|u\|^6) \mathrm{e}^{c + c\|u\|^2} \int_0^t (1 + \|e_1\|^2) \, \|e_1\|_1^2 \, \mathrm{d}\tau.$$

Integrating the above inequality with respect to t_0 in $(0, t)$ we obtain

$$\|e_2(t)\|_s^2 + \nu \int_{t_0}^t \|e_2\|_{1+s}^2 \, \mathrm{d}\tau \leqslant \frac{c}{t_0}(t_0 + 1 + \|u\|^6) \int_0^t (1 + \|e_1\|^2) \, \|e_1\|_1^2 \, \mathrm{d}\tau \quad (5.9)$$

for $t > t_0$.

Now we estimate $\|e_2(t)\|_s$ for $s > 1$. Taking the inner product of (5.6) with $A^{1+l} e_2$, $0 < l < 1$, we obtain

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|e_2\|_{1+l}^2 + \nu \|e_2\|_{2+l}^2 \leqslant |(((e_1 + e_2) \cdot \nabla) v, A^{1+l} e_2)| + |((v^N \cdot \nabla)(e_1 + e_2), A^{1+l} e_2)|.$$

Since (see [5])

$$\big((u \cdot \nabla) v, A^{1+l} w\big) \leqslant c \, \|u\|_{1+l} \, \|v\|_1 \, \|w\|_{2+l} + c \, \|u\|_l \, \|v\|_2 \, \|w\|_{2+l}$$

and using Young's inequality, we can write

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \|e_2\|_{1+l}^2 + \nu \|e_2\|_{2+l}^2 \leqslant {} & c \, \|e_1\|_{1+l}^2 \|v\|_1^2 + c \, \|e_1\|_l^2 \|v\|_2^2 \\ & + c \, \|e_2\|_{1+l}^2 \|v\|_1^2 + c \, \|e_2\|_l^2 \|v\|_2^2 \\ & + c \, \|v^N\|_{1+l}^2 \|e_1\|_1^2 + c \, \|v^N\|_l^2 \|e_1\|_2^2 \\ & + c \, \|v^N\|_{1+l}^2 \|e_2\|_1^2 + c \, \|v^N\|_l^{2/l} \|e_2\|_{1+l}^2. \end{aligned}$$

Now we integrate the above inequality with respect to t and over $(t_0/2+\sigma, t)$ with $0 < t_0 < t$ and $0 < \sigma < t - t_0/2$ and obtain (noting that $\|v^N\|_s \leqslant \|v\|_s$ for any $s > 0$)

$$
\begin{aligned}
\|e_2(t)\|_{1+l}^2 \leqslant{}& \|e_2(t_0/2+\sigma)\|_{1+l}^2 + \sup_{\tau \geqslant t_0/2} \|v(\tau)\|_1^2 \int_{t_0/2+\sigma}^t \|e_1\|_{1+l}^2 + \|e_2\|_{1+l}^2 \,\mathrm{d}\tau \\
&+ \sup_{\tau \geqslant t_0/2} (\|e_1(\tau)\|_l^2 + \|e_2(\tau)\|_l^2) \int_{t_0/2+\sigma}^t \|v\|_2^2 \,\mathrm{d}\tau \\
&+ \sup_{\tau \geqslant t_0/2} (\|e_1(\tau)\|_1^2 + \|e_2(\tau)\|_1^2) \int_{t_0/2+\sigma}^t \|v^N\|_{1+l}^2 \,\mathrm{d}\tau \\
&+ \sup_{\tau \geqslant t_0/2} (1 + \|v^N(\tau)\|_l^{2/l}) \int_{t_0/2+\sigma}^t \|e_1\|_2^2 + \|e_2\|_{1+l}^2 \,\mathrm{d}\tau.
\end{aligned}
$$

We have, for $s > 1$ and $t > t_0$, ([5])

$$
\|v(t)\|_s^2 \leqslant \frac{c(1+\|u\|^4)}{t_0^s}.
$$

Therefore using (5.9) and (5.7) we conclude that

$$
\begin{aligned}
\|e_2(t)\|_{1+l}^2 \leqslant{}& \|e_2(t_0/2+\sigma)\|_{1+l}^2 \\
&+ C_p(\|u\|) \left(\frac{1}{N^{2(m-l)}\, t_0^{1+m}} + \frac{1}{t_0^{1+l}} \int_0^t (1+\|e_1\|^2)\, \|e_1\|_1^2 \,\mathrm{d}\tau + \frac{1}{N^{2(r-1)}\, t_0^{1+r}} \right)
\end{aligned}
$$

with $r > 1$ and where $C_p(\|u\|)$ is a constant depending on polynomials of $\|u\|$. Integrating the above inequality with respect to σ over $(0, t - t_0/2)$ we obtain

$$
\begin{aligned}
\|e_2(t)\|_{1+l}^2 \leqslant{}& C_p(\|u\|) \left(\frac{1}{t_0^{1+l}} + \frac{1}{t_0^{2+l}} \right) \int_0^t (1+\|e_1\|^2)\, \|e_1\|_1^2 \,\mathrm{d}\tau \\
&+ C_p(\|u\|) \left(\frac{1}{N^{2(m-l)}\, t_0^{2+m}} + \frac{1}{N^{2(r-1)}\, t_0^{2+r}} \right).
\end{aligned}
$$

Now to show that $\|e_1\|^2 + \int_0^t \|e_1\|_1^2 \,\mathrm{d}\tau \to 0$ as $N \to \infty$, we note that e_1 satisfies

$$
\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|e_1\|^2 + \nu\|De_1\| &\leqslant \|(I-\mathbb{P}^N)f\|\, \|e_1\| + \|(B(v,v), e_1)\| \\
&\leqslant \|(I-\mathbb{P}^N)f\|\, \|e_1\| + \|v\|^{1/2}\, \|Dv\|^{3/2}\, \|e_1\|^{1/2}\, \|De_1\|^{1/2} \\
&\leqslant \|(I-\mathbb{P}^N)f\|\, \|e_1\| + c\,\|v\|^{2/3}\, \|Dv\|^2\, \|e_1\|^2 + \frac{\nu}{2}\|De_1\|^2.
\end{aligned}
$$

Therefore

$$
\frac{\mathrm{d}}{\mathrm{d}t}\|e_1\|^2 + \nu\|De_1\| \leqslant c\,\|(I-\mathbb{P}^N)f\|^2 + c\,(1+\|v\|^{2/3}\,\|Dv\|^2)\,\|e_1\|^2
$$

and after integrating, we get

$$\|e_1\|^2 + \int_0^T \|e_1\|_1 \, \mathrm{d}\tau \leqslant \exp(1 + C_p(\|u\|)) \left(\|e_1(0)\|^2 + \int_0^T \|(I - \mathbb{P}^N) f\|^2 \right) \mathrm{d}\tau.$$

Since $f \in L^2(0, T; \mathcal{H})$, the above integral tend to zero as $N \to \infty$ and the result follows. □

6 Conclusions

In this paper we have studied the approximation of inverse problems which have been regularized by means of a Bayesian formulation. We have developed a general approximation theory which allows for the transfer of approximation results for the forward problem into approximation results for the inverse problem. The theory clearly separates analysis of the forward problem, in which no probabilistic methods are required, and the probabilistic framework for the inverse problem itself: it is simply necessary that the requisite bounds and approximation properties for the forward problem hold in a space with full measure under the prior. Indeed the approximation theory may be seen to place constraints on the prior, in order to ensure the desired robustness.

In applications there are two sources of error when calculating expectations of functions of infinite dimensional random variables: the error which we provide an analysis for in this paper, namely the approximation of the measure itself in a finite dimensional subspace, together with the error incurred through calculation of expectations. The latter can be undertaken by Markov chain-Monte Carlo (MCMC) methods, or quasi Monte Carlo methods. The two sources of error must be balanced in order to optimize computational cost.

We have studied three specific applications, all concerned with determining the initial condition of a dissipative PDE, from observations of various kinds, at positive times. However the general approach is applicable to a range of inverse problems for functions when formulated in a Bayesian fashion. The article [25] overviews many applications from this point of view. Furthermore we have limited our approximation of the underlying forward problem to spectral methods. However we anticipate that the general approach will be useful for the analysis of other spatial approximations based on finite element methods, for example, and to approximation errors resulting from time-discretization; indeed it would be interesting to carry out analyses for such approximations.

It is important to realize that new approaches to the computation of expectations against measures on infinite dimensional spaces are currently an active area of research in the engineering community [23, 24] and that a numerical analysis of

this area is being systematically developed [22, 29]. That work is primarily concerned with approximating measures which are the push forward, under a nonlinear map, of a simple measure with product strcuture, such as a Gaussian measure; in contrast the inverse problem setting which we study here is concerned with the approximation of non-Gaussian measures whose Radon-Nikodym derivative is defined through a related nonlinear map. It would be interesting to combine the approaches in [23, 22, 29] and related literature with the approximation theories described in this paper. For example that work could be used to develop cheap approximations to the forward map $\mathcal{G}$ thereby accelerating MCMC-based sampling methods.

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Appendix A Analytic Semigroups and Probability

We collect together some basic facts concerning analytic semigroups and probability required in the main body of the article. First we state the well-known Gronwall inequality in the form in which we will use it[4]

Lemma A.1 *Let $I = [c, d)$ with $d \in (c, \infty]$. Assume that $\alpha, u \in C(I; \mathbb{R}^+)$ and that there is $\lambda < \infty$ such that, for all intervals $J \subseteq I$, $\int_J \beta(s)ds < \lambda$. If*

$$u(t) \leqslant \alpha(t) + \int_c^t \beta(s)u(s)ds, \quad t \in I,$$

then

$$u(t) \leqslant \alpha(t) + \int_c^t \alpha(s)\beta(s) \exp\Big(\int_s^t \beta(r)dr\Big)ds, \quad t \in I.$$

In particular, if $\alpha(t) = u + 2at$ is positive in I and $\beta(t) = 2b$ then

$$u(t) \leqslant \exp(2bt)u + \frac{a}{b}\Big(\exp(2bt) - 1\Big), \quad t \in I.$$

Finally, if $c = 0$, and $0 < \alpha(t) \leqslant K$ in I, then

$$u(t) \leqslant K + K\lambda \exp(\lambda), \quad t \in I.$$

Throughout this article A denotes either the Laplacian on a smooth, bounded domain in $\mathbb{R}^d$ with Dirichlet boundary conditions (section 3) or the Stokes operator on $\mathbb{T}^2$ (sections 4 and 5). In both cases A is a self-adjoint positive operator A, densely defined on a Hilbert space $\mathcal{H}$, and the generator of an analytic semigroup. We denote by $\{(\phi_k, \lambda_k)\}_{k\in\mathbb{K}}$ a complete orthonormal set of eigenfunctions/eigenvalues for A in $\mathcal{H}$. We then define fractional powers of A by

$$A^\alpha u = \sum_{k\in\mathbb{K}} \lambda_k^\alpha \langle u, \phi_k\rangle \phi_k. \tag{A.1}$$

For any $s \in \mathbb{R}$ we define the Hilbert spaces $\mathcal{H}^s$ by

$$\mathcal{H}^s = \{u : \sum_{k\in\mathbb{K}} \lambda_k^s |\langle u, \phi_k\rangle|^2 < \infty\}. \tag{A.2}$$

The norm in $\mathcal{H}^s$ is denoted by $\|\cdot\|_s$ and is given by

$$\|u\|_s^2 = \sum_{k\in\mathbb{K}} \lambda_k^s |\langle u, \phi_k\rangle|^2.$$

[4] See `http://en.wikipedia.org/wiki/Gronwall's_inequality`

Of course $\mathcal{H}^0 = \mathcal{H}$. If $s > 0$ then these spaces are contained in $\mathcal{H}$, but for $s < 0$ they are larger than $\mathcal{H}$. It follows that the domain of A^α is $\mathcal{H}^{2\alpha}$; the image of $A^{-\alpha}$ is $\mathcal{H}^{2\alpha}$.

Now consider the Hilbert-space valued ODE

$$\frac{dv}{dt} + Av = f, \quad v(0) = u. \tag{A.3}$$

We state some basic results in this area, provable by use of the techniques in [20], for example, or by direct calculation using the eigenbasis for A. For $f = 0$ the solution $v \in C([0,\infty),\mathcal{H}) \cap C^1((0,\infty), D(A))$ and

$$\|v\|_s^2 \leqslant Ct^{-(s-l)}\|u\|_l^2, \quad \forall t \in (0,T]. \tag{A.4}$$

If $f \in C([0,T],\mathcal{H}^\gamma)$ for some $\gamma \geqslant 0$, then (A.3) has a unique mild solution $u \in C([0,T];\mathcal{H})$ and, for $0 \leqslant \ell < \gamma + 2$,

$$\|v(t)\|_s \leqslant C\Big(\frac{\|u\|_l}{t^{(s-l)/2}} + \|f\|_{C([0,T],\mathcal{H}^\gamma)}\Big) \tag{A.5}$$

for $s \in [\ell, 2+\gamma)$.

It central to this paper to estimate the distance between two probability measures. To this end we introduce two useful metrics on measures: the *total variation distance* and the *Hellinger distance*. We discuss the relationships between the metrics and indicate how they may be used to estimate differences between expectations of random variables under two different measures.

Assume that we have two probability measures μ and μ', both absolutely continuous with respect to the same reference measure ν. The following defines two concepts of distance between μ and μ'.

Definition A.2 *The* total variation distance *between μ and μ' is*

$$d_{\mathrm{TV}}(\mu,\mu') = \frac{1}{2}\int\Big|\frac{d\mu}{d\nu} - \frac{d\mu'}{d\nu}\Big|d\nu.$$

The Hellinger distance *between μ and μ' is*

$$d_{\mathrm{Hell}}(\mu,\mu') = \sqrt{\Big(\frac{1}{2}\int\Big(\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}}\Big)^2 d\nu\Big)}.$$

Both distances are invariant under the choice of ν in that they are unchanged if a different reference measure, with respect to which μ and μ' are absolutely continuous, is used. Furthermore, it follows from the definitions that $d_{\mathrm{TV}}(\mu,\mu') \in (0,1)$

and $d_{\text{Hell}}(\mu,\mu') \in (0,1)$. The Hellinger and total variation distances are related as follows[9][5]:

$$\frac{1}{\sqrt{2}} d_{\text{TV}}(\mu,\mu') \leqslant d_{\text{Hell}}(\mu,\mu') \leqslant d_{\text{TV}}(\mu,\mu')^{\frac{1}{2}}. \tag{A.6}$$

The Hellinger distance is particularly useful for estimating the difference between expectation values of functions of random variables under different measures. This is illustrated in the following lemma:

Lemma A.3 *Assume that two measures μ and μ' on a Banach space $\Big(X, \|\cdot\|_X\Big)$ are both absolutely continuous with respect to a measure ν. Assume also that $f : X \to Z$, where $\Big(Z, \|\cdot\|\Big)$ is a Banach space, has second moments with respect to both μ and μ'. Then*

$$\|\mathbb{E}^{\mu} f - \mathbb{E}^{\mu'} f\| \leqslant 2\Big(\mathbb{E}^{\mu}\|f\|^2 + \mathbb{E}^{\mu'}\|f\|^2\Big)^{\frac{1}{2}} d_{\text{Hell}}(\mu,\mu').$$

Furthermore, if $\Big(Z, \langle\cdot,\cdot\rangle\Big)$ is a Hilbert space and $f : X \to Z$ has fourth moments then

$$\|\mathbb{E}^{\mu} f\otimes f - \mathbb{E}^{\mu'} f\otimes f\| \leqslant 2\Big(\mathbb{E}^{\mu}\|f\|^4 + \mathbb{E}^{\mu'}\|f\|^4\Big)^{\frac{1}{2}} d_{\text{Hell}}(\mu,\mu').$$

Proof. We have

$$\begin{aligned}
\|\mathbb{E}^{\mu} f - \mathbb{E}^{\mu'} f\| &\leqslant \int \|f\| \Big|\frac{d\mu}{d\nu} - \frac{d\mu'}{d\nu}\Big| d\nu \\
&\leqslant \int \Big(\frac{1}{\sqrt{2}}\Big|\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}}\Big|\Big)\Big(\sqrt{2}\|f\|\Big|\sqrt{\frac{d\mu}{d\nu}} + \sqrt{\frac{d\mu'}{d\nu}}\Big|\Big) d\nu \\
&\leqslant \sqrt{\Big(\frac{1}{2}\int\Big(\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}}\Big)^2 d\nu\Big)}\sqrt{\Big(2\int \|f\|^2\Big(\sqrt{\frac{d\mu}{d\nu}} + \sqrt{\frac{d\mu'}{d\nu}}\Big)^2 d\nu\Big)} \\
&\leqslant \sqrt{\Big(\frac{1}{2}\int\Big(\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}}\Big)^2 d\nu\Big)}\sqrt{\Big(4\int \|f\|^2\Big(\frac{d\mu}{d\nu} + \frac{d\mu'}{d\nu}\Big) d\nu\Big)} \\
&= 2\Big(\mathbb{E}^{\mu}\|f\|^2 + \mathbb{E}^{\mu'}\|f\|^2\Big)^{\frac{1}{2}} d_{\text{Hell}}(\mu,\mu')
\end{aligned}$$

as required.

[5]Note that different normalization constants are sometimes used in the definitions of distance.

The proof for $f \otimes f$ follows from the following inequalities, and then arguing similarly to the case for the norm of f:

$$\begin{aligned}\|\mathbb{E}^{\mu} f \otimes f - \mathbb{E}^{\mu'} f \otimes f\| &= \sup_{\|h\|=1} \|\mathbb{E}^{\mu}\langle f, h\rangle f - \mathbb{E}^{\mu'}\langle f, h\rangle f\| \\ &\leqslant \int \|f\|^2 \Big|\frac{d\mu}{d\nu} - \frac{d\mu'}{d\nu}\Big| d\nu.\end{aligned}$$

□

Note, in particular, that choosing $X = Z$, and with f chosen to be the identity mapping, we deduce that the differences in mean and covariance operators under two measures are bounded above by the Hellinger distance between the two measures.

The following Fernique Theorem (see [21], Theorem 2.6) will be used repeatedly:

Theorem A.4 *Let $x \sim \mu = \mathcal{N}(0, \mathcal{C})$ where μ is a Gaussian measure on Hilbert space H. Assume that $\mu_0(X) = 1$ for some Banach space $\Big(X, \|\cdot\|_X\Big)$ with $X \subseteq H$. Then there exists $\alpha > 0$ such that*

$$\int_{\mathcal{H}} \exp(\alpha \|x\|_X^2)\mu(dx) < \infty.$$

The following regularity properties of Gaussian random fields will be useful to us; the results may be proved by use of the Kolmogorov continuity criterion, together with the Karhunen-Loeve expansion (see [21], section 3.2):

Lemma A.5 *Consider a Gaussian measure $\mu = \mathcal{N}(0, \mathcal{C})$ with $\mathcal{C} = \beta A^{-\alpha}$ where A is as defined earlier in this Appendix A. Then $u \sim \mu$ is almost surely $s-$Hölder continuous for any exponent $s < \min\{1, \alpha - \frac{d}{2}\}$ and $u \in \mathcal{H}^s$, $\mu-$almost surely, for any $s < \alpha - \frac{d}{2}$.*